Thiamine disulfide
67-16-3 | DTXSID6046890

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 175 °C

Global applicability domain: Outside

Local applicability domain index: 2.10e-01

Confidence level: 6.86e-01

Nearest Neighbors from the Training Set

Image not found
Thiamine disulfide
Measured: 177
Predicted: 175

Image not found
Bisbentiamine
Measured: 147
Predicted: 149

Image not found
Puromycin
Measured: 176
Predicted: 176

Image not found
Dipyridamole
Measured: 163
Predicted: 164

Image not found
Mopidamol
Measured: 158
Predicted: 164